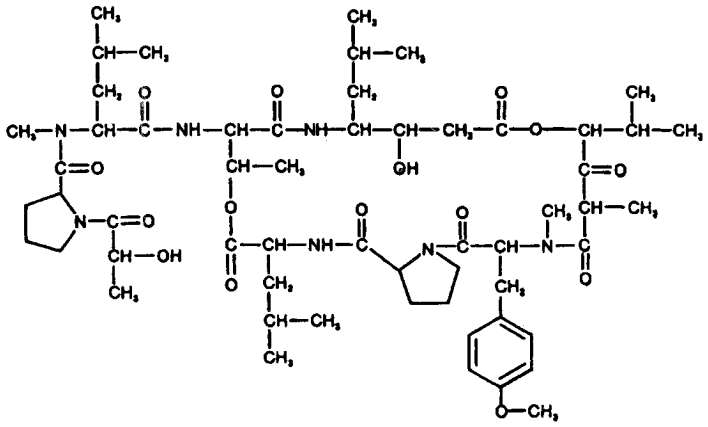
DIDEMNIN B

NSC - 325319



Chemical Name: *N*-[1-[*N*-[4-[[3-Hydroxy-4-[[*N*-[*N*-[1-(2-hydroxy-1-oxopropyl)-*L*-prolyl]-*N*-methyl-*L*-leucyl]-*L*-threonyl]amino-5-methyl-1-oxoheptyl]oxy]-2,5-dimethyl-1,3-dioxohexyl]-*L*-leucyl]-*L*-prolyl]-*N*,*O*-dimethyl-*L*-tyrosine, ϕ-lactone

CAS Registry Number: 77327-05-0

Molecular Formula: $C_{57}H_{89}N_7O_{15}$ **M.W.:** 1112.0

Approximate Solubility:	(mg/mL)
H_2O	< 0.1
CH_3OH	> 100
$CHCl_3$	> 100
DMSO	> 100
C_2H_5OH	> 100
CH_2Cl_2	> 100

Stability:

Bulk:
As a bulk chemical, didemnin B is found to be stable at 25 ± 2 °C for 3 weeks. At the end of 4 weeks, approximately 2% decomposition has occurred.
When stored at 45 °C, didemnin B appeared stable for 2 weeks; after this time, it slowly decomposed to an approximate 7% loss at the end of 4 weeks (HPLC).

Solution:
As a 6 mg/mL 50% aqueous ethanol solution at room temperature (25 ± 2 °C) didemnin B appeared stable for at least 26 hours (HPLC).

Ultraviolet Absorption:

(MeOH)

λ_{max}	ε
284 ± 2 nm(sh)	1,455 - 1,490
277 ± 2 nm	1,705 - 1,750
220 ± 2 nm(sh)	17,500 - 19,199
205 ± 2 nm	29,100 - 29,700

High Performance Liquid Chromatography:

Column:	Whatman Partisil 5 ODS, 250 mm x 4.6 mm i.d.
Mobile Phase:	CH_3OH/H_2O/triethylamine, 75/25/0.01 (adjusted to pH 7.5 with acetic acid)

Flow Rate:	1.0 mL/min
Detection:	UV at 275 nm
Sample Preparation:	3 mg/mL in internal standard solution
Internal Standard:	1 mL hexaphenone per liter methanol
Retention Volume:	19 mL (NSC-325319) 10 mL (I.S.)

Toxicity Data:

Rat(iv): LD_{50}: 860 μg/kg
National Technical Information Service, PB84-192251

Mouse(iv): LD_{50}: 1530 μg/kg
National Technical Information Service, PB84-192251

Dog (iv): LD50: 418 g/kg
National Technical Information Service, PB84-192251